

CENTENARY REVIEW

The circuitous path to the comparison of simulated values from crop models with field observations

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(Revised MS received 10 August 2006; First published online 12 October 2006)

SUMMARY

The *Journal of Agricultural Science, Cambridge* has been a fixture in dissemination of crop simulation models and the concepts and data upon which they are built since the inception of computers and computer modelling in the mid-20th century. To quantify the performance of a crop simulation model, model outputs are compared with observed values using statistical measures of bias, i.e. the difference between simulated and observed values. While applying these statistical measures is unambiguous for the experienced user, the same cannot always be said of determining the observed or simulated values. For example, differences in accessing crop development can be due to the subjectivity of an observer or to a definition that is difficult to apply in the field. Methods of determining kernel number, kernel mass, and yield can vary among researchers, which can add errors to comparisons between experimental observations and simulated results. If kernel moisture is not carefully determined and reported it can add error to values of grain yield and kernels per unit area regardless of the protocol used to collect these data. Inaccurate determination of kernel moisture will also influence computation of grain protein or oil content. Problems can also be associated with input data to the simulation models. Under-reporting of precipitation values from tipping bucket rain gauges, commonly found on automated weather stations, can introduce errors in results from crop simulation models. Using weather data collected too far from an experimental site may compound problems with input data. The importance of accurate soil and weather input data increases as the environment becomes more limiting for plant growth and development. Problems can also arise from algorithms that calculate important parameters in a model, such as daylength, which is used to determine a photoperiod response. Errors in the calculation of photoperiod can be related to the definition of sunrise and sunset and the inclusion or exclusion of civil twilight or to the improper calculation of the solar declination. Even the simple calculation of the daily mean air temperature can have an impact on the results from a non-linear algorithm. During a period when crop simulation modelling is moving in the difficult direction of incorporating genomic-based inputs, the critical importance of careful and accurate collection and reporting of field data and the need to develop robust algorithms that accommodate readily available or easily acquired input data should not be forgotten. As scientists we have an obligation to provide the best available knowledge and understanding as possible. Avoiding potential pitfalls will assist us as we develop new knowledge and understanding and incorporate these concepts into new or modified crop simulation models.

INTRODUCTION

One hundred years in geological time is miniscule, passing without perceptible change. In contrast, 100 years in the life of a scientific journal represents an

exceptionally long period, characterized by enormous changes in technology, while fundamental problems remain surprisingly similar. As noted in the editorial that began the 100th anniversary volume (Volume 143) of the *Journal of Agricultural Science, Cambridge* (JAS), issues addressed in the first volume resonate in current articles. The first paper in Volume 1 (Biffen

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1905) discussed the necessity of improving grain end-use quality of British grown wheat through breeding. There was an economic incentive to use solely British wheat, rather than blend this with imported wheat, to produce flour with the required end-use quality characteristics. Other papers in the inaugural issue presented observations on soil management techniques to improve plant growth, to change crop composition, to follow movement of plant nutrients in the environment, and to understand the influence of environment and genetics on crop growth and yield. Papers with similar themes have appeared in recent volumes of JAS, but techniques used have changed greatly from Volume 1 to Volume 144. Crop simulation modelling is one of the new techniques.

Simulation models in agriculture, used as tools for both forecasting and understanding, were developed soon after the first commercial computers became available. An integral part of the development of these models was field observations designed to fill knowledge gaps. Table 1 lists many of the papers that were published in JAS regarding crop models and the observational studies upon which they are based. This list is not exhaustive, but an indication of the wide variety of modelling papers published in JAS. While many papers discuss the problems and concerns associated with model development, the pitfalls involved with model development and assessment have not received as much attention.

A necessary component in the evaluation of a crop simulation model is the comparison of observed and simulated values. This comparison can be quantified using a statistical measure of central tendency and dispersion. That is, measures of the mean and variance. Combinations of these measures, such as mean error, mean absolute error, root mean square error, normalized root mean square error, index of agreement, and modelling efficiency are frequently used (Janssen & Heuberger 1995). Following this analysis, there is usually an explanation of why the simulated results occurred. When large differences occur between simulated and observed values, a conclusion may be reached that a process is not well understood and further experimental work is required to quantify the variables associated with a process. Conversely, favourable comparisons may imply that a process is satisfactorily understood for that particular modelling application. However, there may be situations where either good or poor agreement between simulated and observed values results from an error in an observation or in the use of an input variable in the simulation model. While one may be able to evaluate the strengths and weaknesses (assumptions) of an algorithm, problems associated with observational errors may be subtle. Similar types of errors may also be associated with model input data. One could easily argue that there are errors in all data and these errors

are well known and dealt with by the appropriate experimental and simulation protocols usually described in the Materials and Methods section of a manuscript. In response, one might contend that serious errors can occur when we assume that protocols for measurement procedures for specific parameters are common knowledge and are consistent for a crop, a discipline, or a period of time.

A technological example to illustrate the latter point occurred on 23 September 1999, when the NASA Climate Orbiter crashed, rather than orbited Mars, because one engineering group used English units and another SI units for a key spacecraft operation. A simulation example is provided in McMaster & Wilhelm (1997) where two accepted methods of calculating thermal time are evaluated, resulting in different values of accumulated thermal time with the same data set. In describing some of these measurement protocols important details may not be adequately explained, which can result in others who follow these protocols making inappropriate assumptions. Carberry (1991) corrected algorithms to simulate leaf area in maize (*Zea mays* L.) based on initial misinterpretation of parameter definitions in the published documentation of the model. Published algorithms may contain errors. For example, the equation relating phyllochron to daylength at time of crop emergence presented by Baker *et al.* (1980) contained an error (the slope of the linear relationship was transposed, it was published as 0.62 when it should have been 0.26 per degree day) as noted by McMaster *et al.* (1991). Though errata and associated correspondence may be published, they may be difficult to locate unless one is a constant reader of the same journal. Furthermore, additional commentary on an article may cause more confusion rather than enhance understanding.

An interesting example of this phenomenon is the publication by Walraven (1978) on the calculation of the elevation and azimuth angles of the sun, which was based on simplified astronomical calculations, with a stated accuracy of $\pm 0.01^\circ$. That paper was followed by a series of comments and comments on comments: Walraven (1979), Archer (1980), Wilkinson (1981), Muir (1983), Wilkinson (1983), Ilyas (1983), Pascoe (1984), Ilyas (1984*a*), Wilkinson (1984), Ilyas (1984*b*), Kambezidis & Papanikolaou (1990), and Kambezidis & Tsangrassoulis (1993). In an attempt to clarify the confusion caused by the first 10 papers, Michalsky (1988*a*) published a series of algorithms with the same stated accuracy as in Walraven (1978). This publication was followed by Michalsky (1988*b*), Spencer (1989), and Michalsky (1989) in order to correct and clarify some components of this 'corrected' algorithm.

Workers, who may not appreciate the detail that is required for accurate field-related measurements, may make the majority of these measurements. While

Table 1. *Observational studies supporting crop modelling and crop modelling studies published in JAS from 1970 through 2006 (Volumes 74–144). See References for full details*

Author	Year	Title
Observational studies		
Willey & Holliday	1971	Plant population and shading studies in barley.
Kirby & Faris	1972	The effect of plant density on tiller growth and morphology in barley.
Kirby	1974	Ear development in spring wheat.
Hadjichristodoulou <i>et al.</i>	1977	Effect of sowing depth on plant establishment, tillering capacity and other agronomic characters of cereals.
Dale & Wilson	1978	A comparison of leaf and ear development in barley cultivars as affected by nitrogen supply.
Gallagher & Biscoe	1978	Radiation absorption, growth and yield of cereals.
Gregory <i>et al.</i>	1978 <i>a</i>	Water relations in winter wheat: 2. Soil water relations.
Gregory <i>et al.</i>	1978 <i>b</i>	Water relations of winter wheat: 1. Growth of the root system.
Legg <i>et al.</i>	1979	The effects of drought on barley growth: Models and measurements showing the relative importance of leaf area and photosynthetic rate.
Gregory <i>et al.</i>	1981	Nutrient relations in winter wheat. 3. Nitrogen uptake, photosynthesis of flag leaves and translocation of nitrogen to grain.
Austin	1982	Crop characteristics and the potential yield of wheat.
Barraclough	1984	The growth and activity of winter wheat roots in the field: Root growth of high-yielding crops in relation to shoot growth.
Gregory <i>et al.</i>	1984	Effects of fertilizer on root growth and water use of barley in northern Syria.
McGowan <i>et al.</i>	1984	Water relations of winter wheat. 5: The root system and osmotic adjustment in relation to crop evaporation.
Singh <i>et al.</i>	1984	Physiological maturity in <i>Aestivum</i> wheat: visual determination.
Fischer	1985	Number of kernels in wheat crops and the influence of solar radiation and temperature.
Kirby <i>et al.</i>	1987	An analysis of primordium initiation in Avalon winter wheat crops with different sowing dates and at nine sites in England and Scotland.
Porter <i>et al.</i>	1987	An analysis of morphological development stages in Avalon winter wheat crops with different sowing dates and at ten sites in England and Scotland.
Thorne & Wood	1988	Contributions of shoot categories to growth and yield of winter wheat.
Kirby	1992	A field study of the number of main shoot leaves in wheat in relation to vernalization and photoperiod.
Cousens <i>et al.</i>	1993	Comparative rates of emergence and leaf appearance in wild oats (<i>Avena fatua</i>), winter barley (<i>Hordeum sativum</i>), and winter wheat (<i>Triticum aestivum</i>).
Kirby <i>et al.</i>	1994	Coordination of stem elongation and Zadoks growth stages with leaf emergence in wheat and barley.
Kernich <i>et al.</i>	1995	Barley development as affected by rate of change of photoperiod.
Moot <i>et al.</i>	1996	Rate of change in harvest index during grain-filling of wheat.
Slafer	1996	Differences in phasic development rate amongst wheat cultivars independent of responses to photoperiod and vernalization. A viewpoint of the intrinsic earliness hypothesis.
Mulholland <i>et al.</i>	1997	Timing of critical developmental stages and leaf production in field-grown spring wheat for use in crop models.
Gillett <i>et al.</i>	2001	An approach to modelling the effect of environmental and physiological factors upon biomass accumulation in winter wheat.
Smith <i>et al.</i>	2002	EuroSOMNET – a European database of long-term experiments on soil organic matter.
Modelling studies		
Barnes <i>et al.</i>	1976	A dynamic model for the effects of potassium and nitrogen fertilizers on the growth and nutrient uptake of crops.
Greenwood & Barnes	1978	A theoretical model for the decline in the protein content in plants during growth.
Thompson	1981	Modelling the field drying of hay.
Towner	1983	A theoretical examination of Burns' (1975) equation for predicting the leaching of nitrate fertilizer applied to a soil surface.
Porter	1984	A model of canopy development in winter wheat.
Weir <i>et al.</i>	1984	A winter wheat crop simulation model without water or nutrient limitations.
Addiscott & Whitmore	1987	Computer simulation of changes in soil mineral nitrogen and crop nitrogen during autumn, winter and spring
Travis	1987	Use of a simple model to study factors affecting the size distribution of tubers in potato crops.
Pal <i>et al.</i>	1990	Simple water-balance models for simulating moisture, salinity, and sodicity profiles in soil under wheat.

Table 1 (cont.)

Author	Year	Title
Firman <i>et al.</i>	1992	Predicting the emergence date of potato sprouts
McMaster <i>et al.</i>	1992	Simulating winter wheat shoot apex phenology.
Bradbury <i>et al.</i>	1993	Modelling the fate of nitrogen in crop and soil in the years following application of ¹⁵ N-labelled fertilizer to winter wheat.
Kocabas <i>et al.</i>	1993	Sensitivity analyses of the ARCWHEAT1 crop model: The effects of changes in radiation and temperature.
Benbi	1994	Prediction of leaf area indices and yield of wheat.
Hamer <i>et al.</i>	1994a	Crop production and water-use. II. The development and validation of a water-use model for sugarbeet.
Hamer <i>et al.</i>	1994b	Crop production and water-use. III. The development and validation of a water-use model for potato.
Siddons <i>et al.</i>	1994	The use of a land suitability model to predict where autumn-sown, determinate genotypes of the white lupin (<i>Lupinus albus</i>) might be grown in England and Wales.
Wright <i>et al.</i>	1994	Crop production and water-use. I. A model for estimating crop water-use with limited data.
Brignall & Rownsevell	1995	Land evaluation modelling to assess the effects of climate change on winter wheat potential in England and Wales.
Craigon <i>et al.</i>	1995	Modelling the effects of vernalization on progress to final leaf appearance in winter wheat.
Hamer	1995	Modelling the effects of sowing date and plant density on the yield and timing of development of Brussels sprouts (<i>Brassica oleracea</i>).
Cao & Moss	1997	Modelling phasic developments in wheat: a conceptual integration of physiological components.
Kirby & Wrightman	1997	Discrepancies between observed and predicted growth stages in wheat.
Weightman <i>et al.</i>	1997	Prediction of leaf and internode development in wheat.
Wright <i>et al.</i>	1997	Crop production and water-use. IV. Yield function for sugar beet.
Phillips <i>et al.</i>	1998	A basis for predictive modelling of the relationship of the potato yield to population density of potato cyst nematode, <i>Globodera pallida</i> .
Kaur & Hundal	1999	Forecasting growth and yield of groundnut (<i>Arachis hypogaea</i>) with a dynamic simulation model 'PNUTGROW' under Punjab conditions
Keady <i>et al.</i>	2000	Prediction of silage feeding value from the analysis of the herbage at ensiling and effects of nitrogen fertilizer, date of harvest and additive treatment on grass silage composition.
Kebreab <i>et al.</i>	2000	An evaluation of uptake and developmental impact in the semi-arid tropics of four crop production models.
Wurr <i>et al.</i>	2000	Climate change, a response surface study of the effects of CO ₂ and temperature on the growth of French beans.
Cheyglinted <i>et al.</i>	2001	Assessment of the CERES-rice model for rice production in the central plain of Thailand.
Gabrielle <i>et al.</i>	2001	Ability of the SUNDIAL model to simulate the short-term dynamics of ¹⁵ N applied to winter wheat and oilseed rape.
Ntare <i>et al.</i>	2001	Evaluation of groundnut genotypes for heat tolerance under field conditions in a Sahelian environment using a simple physiological model for yield.
Kage <i>et al.</i>	2003	Aspects of nitrogen use efficiency of cauliflower I. A simulation modelling based analysis of nitrogen availability under field conditions.
Lombnaes & Singh	2003	Predicting Zn and Cu status in cereals – potential for a multiple regression model using soil parameters.
McMaster & Wilhelm	2003	Phenological responses of wheat and barley to water & temperature: improving simulation models.
Zahedi & Jenner	2003	Analysis of effects in wheat of high temperature on grain filling attributes estimated from mathematical models of grain filling.
Nain <i>et al.</i>	2004	Use of CERES-wheat model for wheat yield forecast in central Indo-Gangetic Plains of India.
Holst	2005	Recursive density equivalents: An improved method for forecasting yield loss caused by mixed weed populations.

there may be fewer potential difficulties associated with input data to crop simulation models, care must still be exercised in order to avoid problems. The objective of the present paper is to discuss many of the

potential errors associated with field observations, input data and simulation algorithms. These potential errors are presented with examples from personal experience and the literature. The present authors'

purpose is not to give detailed methods for avoiding these errors (likely an impossible task because solutions are situation specific), but rather to alert the modelling community how seemingly logical and benign assumptions can spawn misleading, and sometimes embarrassing, conclusions and outcomes. To rephrase a quote attributed to the late US Senator Everett Dirksen when discussing budget concerns ('a billion here, a billion there and pretty soon you are talking about real money'), substitute 'error' in the appropriate places in the above statement and the result could be a relatively large error.

FIELD OBSERVATIONS

The ability to simulate plant development is an important component of any crop simulation model because different growth processes occur at different times in the development of a plant. Measurements of plant development present a series of challenges, in part because of their subjective nature; they may differ from observer to observer. Scales to compare non-destructive field observations with defined stages of plant development help minimize this subjectivity. Scales have been created by Feeke (Large 1954) and Zadoks *et al.* (1974) for cereal crops. Similarly, scales for maize and soybean (*Glycine max* (L.) Merr.) have been prepared by Ritchie *et al.* (1997*a,b*). In cereal crops, stages such as single and double ridge require destructive sampling and observation under a powerful hand lens. Although physiological maturity is clearly defined in the Zadoks scale, as when a thumbnail can no longer dent a kernel, this measure is not often used when there are many plots to evaluate because of time considerations in sampling many plants. Hanft & Wych (1982) evaluated 13 methods to determine physiological maturity and found the most practical method to be the complete loss of green colour from the glumes of the lower spikelets. On the other hand, leaf appearance rate determined by the Haun stage (Haun 1973) is less subjective than determining development stages because actual measurements of leaf length can be used to compute this stage.

Measurements of plant development should be made every 2–3 days, but are frequently made at intervals of 7–14 days. In addition, to conserve space in published reports, development stages are reported at less frequent intervals or in figures that may be difficult to accurately interpret. Under certain meteorological conditions, it may be possible for plants to stay at the same stage of development for extended periods. The present authors have observed this situation in wheat (*Triticum aestivum* L.) where the plants remained at the single ridge stage for about 10 days.

Grain yield on a land area basis can be determined either by machine or hand harvesting; each

Table 2. Yield estimate for combine and hand harvested plots

Hybrid	Nitrogen rate (kg N/ha)	Yield (t/ha)	
		Combine	Hand
P3394	0	6.38	7.20
	70	8.19	9.77
	140	8.57	11.15
	210	9.57	12.14
Mean		8.18	10.06
P33A14	0	7.22	8.05
	70	9.09	11.34
	140	10.29	13.23
	210	11.14	13.65
Mean		9.44	11.57

method has advantages and disadvantages. Machine harvesting allows the entire plot or large area to be sampled, minimizing any concerns about plant-to-plant differences within the plot. There are losses, however, associated with machine harvesting. On a well-maintained combine with a skilled operator, one can assume a proportional yield loss of 0.03 for wheat (Anonymous 2003) but a 0.05–0.10 loss for sorghum (*Sorghum bicolor* (L.) Moench; Donald & Ogburn 1982) and as high as 0.30–0.50 for machine harvested amaranth (*Amaranthus* spp. Amaranthaceae; Fitterer *et al.* 1996). On combines that are not well maintained or not operated skillfully, losses can be much greater. Crop simulation models report simulated yield with no assumption of harvest losses.

Hand harvesting eliminates some of these problems, but substitutes other problems: the need to select a representative sample and large enough sample size. Hand harvesting is a time-consuming process, which requires a disciplined labour force. Errors associated with loss of grain or measurement of sample area can also occur with hand harvest methods. Hand harvesting allows determination of the mass of individual plant components (leaves, sheaths, stems and reproductive organs) and leaf area index.

To further exacerbate the problem, if both machine and hand harvest are conducted, results seldom agree though they should be highly correlated. A subset of data from an N response study conducted to determine the impact of several controlled-release formulations of N fertilizer on maize grain yield in the Central Platte Valley of Nebraska, illustrates this problem (Table 2). Mean yield estimates for both hybrids were about 2 t/ha greater with hand harvesting than with machine harvesting. Even though additional N increased yield, differences between the harvest methods remained. In fact, standard errors, F-values, and probabilities of a greater F for hybrid,

N rate, and their interaction were similar for the two harvest methods (data not shown). Combine and hand harvest yield data were highly correlated ($r = 0.81$, $n = 96$). The conclusion about the effects of treatments would be similar for both harvest methods; only the absolute estimates of grain yield differed. If these observed yield values were compared to simulated values, which set of observed values should be used in this comparison?

Mean kernel mass (mg/kernel) is usually based on the mass of some specified or known number of kernels (usually 200–1000). Dividing mean kernel mass into yield provides one estimate of the mean kernel number per unit area. Care must be exercised in using this approach to ensure that the moisture content of the kernel is taken into account, as well as the moisture content of the grain yield estimates. Depending on storage conditions and time between measurement of grain yield and kernel mass, the moisture content difference can be substantial. Simulated values of mass are usually based on a zero moisture content, but field data are usually adjusted to grain marketing standards, i.e. a water content of 155 g/kg for maize, based on estimates of field moisture content that can be determined in several ways (oven drying, moisture meter, etc.) with several sources of error associated with each method. Most newer research combines are equipped with automated scale and moisture meter systems; for accurate readings these metered systems obviously must be well maintained and calibrated. (Proper maintenance and calibration applies to all sensors, which again is obvious, but should be restated.) Even under optimum conditions the grain will never dry to zero moisture, but perhaps to 30 g/kg for wheat, then a grain moisture meter can be used to estimate the correction necessary to bring the mass to the equivalent of zero moisture, again assuming the meter is accurately calibrated.

The above measurement methodologies are appropriate given that most crop simulation models predict mean kernel number and mean kernel mass. These mean values would probably differ from values determined by direct, individual measurements. Furthermore, if one determined the individual components of yield from plot samples (for wheat; plants per unit area, culms per plant, kernels per culm, and individual kernel mass) and multiplied them together; the result may not equal the machine-harvested yield due to variability. Thus, there can be two 'correct' answers regarding yield components.

Kernel moisture also plays an important role in determining component content, such as protein content of the grain, which is usually estimated as the ratio of the kernel nitrogen mass divided by the kernel mass, and the resulting quantity multiplied by a constant (5.7). In this case, the greater the moisture content of the grain, the lower the protein content since the kernel mass is in the denominator of this ratio. If

appropriate corrections for grain water content are not made, observed and simulated results should disagree. A similar argument can be made for oil content of grain or seed. Again, depending upon the question being asked the disagreement will either be trivial or significant.

Moisture is also an important factor when considering radiation (or light) use efficiency, defined as the amount of dry matter formed (above ground or total) per unit of radiation (solar or PAR) absorbed (or intercepted) for a defined time interval. As with all dry matter sampling, care must be exercised to minimize or eliminate loss of sample mass during processing. Leaves and flower parts dry more rapidly than stems and are easy to lose as samples or sample bags are moved, handled and weighed. When using published values of yield and yield components in order to evaluate a crop simulation model, it is important to take into account the moisture content of these values in the comparisons. Field sampling losses are not reported in most cases.

Harvest index (HI), the ratio of grain yield to total above-ground biomass, is frequently used to determine grain yield from simulated total above-ground biomass. Harvest index is also frequently reported for field experiments. Although the definition and computation of HI is straightforward, errors may arise in its calculation. If grain is reported at 155 g water/kg, and total above-ground biomass is reported as dry matter, the resulting estimate of HI based on field measurements will be greater than a simulated value. If HI is computed from values in tables and text of published papers, grain and total above-ground biomass may not have been sampled at the same time, introducing a similar type of error, that is, numerator and denominator are at different moisture contents. Ideally, measurements of grain and above-ground dry matter should be done at the same time, but they may not be. To wait until the grain is dry enough to harvest means that above-ground components may be lost. On the other hand, if one harvests at physiological maturity, when above-ground biomass is at a maximum, the moisture content of the grain is too high for efficient mechanical harvesting. There is a high probability that harvesting at this time would result in much grain loss. In variety trials there would be an argument for harvesting each variety when it becomes mature (to mimic what a grower would do) rather than harvest all varieties at the same time. In addition to the above, one has to consider hand versus machine harvesting and the impact of the different cutting heights associated with each method, on estimates of plant biomass. Frequently hand harvested material is cut near ground level in order to permit later measurement and analysis of plant components. If plant dry mass from machine harvest procedures is used, it may underestimate the allocation to above-ground biomass, which

will affect the computation of harvest index. Using a field-determined value or a published derived value of HI as a component of a simulation model may introduce errors in the simulated yield.

Results of yield trials of different genotypes can be a good source of data to evaluate crop simulation models. While a data set based on yield trials may contain sowing, anthesis, and dates of physiological maturity and yield components, it usually does not contain plant population density (plants/m²). Plant population density is an important input parameter for many crop simulation models and can be estimated by dividing the seeding rate (g/m²) by the kernel dry mass (mg) and assuming some fraction of the seeds germinated and emerged. Unfortunately, this calculation combines several assumptions; that the seeding rate was known and accurately reported and was uniform across genotypes, that kernel mass (which is usually not reported) was accurately estimated, and that the fraction of seeds germinating, emerging, and surviving to maturity were estimated with accuracy.

INPUT DATA

Automated weather stations (which usually measure air temperature, solar radiation, precipitation, relative humidity, wind speed, wind direction, and other parameters) are an essential source of data for crop simulation models. Maintenance of sensors may not be possible on a frequent basis because of the time to travel to a site and problems with sensors are usually identified using quality control techniques. In addition, sensors may have limitations that only become apparent under extreme conditions, such as the non-linearity of the tipping rate of tipping bucket rain gauges and rainfall intensity when, under high rainfall conditions, the bucket cannot tip fast enough to capture all rainfall during intense events. In a simulation study, Heinemann *et al.* (2002) showed that negatively biased precipitation values, i.e. values less than the mean observed values, from tipping bucket rain gauges reduced simulated yields for four crops (maize, wheat, soybean and peanut (*Arachis hypogaea* (L.)), soybean having the largest decrease (19%) in simulated yield and wheat the least, in fact showing a very slight increase (0.2%). Yield responses were more sensitive to negative rather than positive biased precipitation values. Data for the Heinemann *et al.* (2002) study came from Tifton, Georgia, USA, which has an annual mean total precipitation of 1122 mm. For regions with half of this amount of precipitation, errors in rain gauge measurements would probably amplify these results. The message from that study, as well as the other studies cited in the present paper, is to be sensitive to potential sensor errors when analysing simulation model output data.

Aggarwal (1995) studied the outputs of a crop simulation model based on uncertainties in crop, weather and soil inputs represented by statistical distributions of the input parameters. 'Uncertainties' in the outputs increased as the environments changed from one limited only by temperature and radiation (potential), to an irrigated environment, to one limited by water and nitrogen (rainfed). The resulting bias from the first two environments was similar. A way to deal with the uncertainties of the output data associated with input data uncertainties was to have fixed soil and crop inputs run with a long series of weather data. Variables associated with simulating photosynthesis and leaf area were important in the first two systems, and soil nitrogen and vapour pressure inputs were important in the irrigated system. In the rainfed system, soil and weather inputs were more important than crop inputs.

Soil name and classification are often reported in the literature for field sites based solely on location and defined soil series from published data (i.e. soil survey reports), rather than from field measurements. Modellers must assume the soil at the site meets the mean characteristics for the soil, when in fact the soil may only marginally meet the classification criteria for the stated soil and therefore have different characteristics (e.g. pH, particle size distribution, organic matter content, etc.) than a soil meeting the central trend of the stated soil. Individually these differences may have a small influence on the simulated output, but taken together their impact may be relatively large.

Gijsman *et al.* (2003) examined the use of eight algorithms to generate values for drained upper limit (DUL) and lower limit (LL) of plant-available water (values widely used in crop simulation models to define the amount or volume of water held in the soil that can be extracted by plants). These values can be determined experimentally, but the procedures are time consuming and tedious. In addition, empirical determinations require direct access to soils under investigation. In many simulation studies, investigators do not have access to the soil, or the soil under the conditions, in question. In these circumstances, derivation of DUL and LL may be the only reasonable alternative. Unfortunately, the thorough sensitivity analysis performed by Gijsman *et al.* (2003) indicated that none of the methods for computing DUL and LL from the more readily available soil texture data, proved acceptable over the entire range of textural classes. However, the method described in Saxton *et al.* (1986) performed the best of the methods investigated in this study, except for very sandy soils where no model performed well. Additionally, Gijsman *et al.* (2003) highlight what they call a 'worrysome lack of accuracy in presentation of methods in articles'. They continue, stating: 'This means that among the many methods available

Table 3. Length of record, elevation, mean annual daily minimum and maximum temperatures, and mean annual total precipitation for Astoria, Oregon and Bishop, California, USA

Location and length of record	Elevation (m)	Mean annual daily minimum temperature (°C)	Mean annual daily maximum temperature (°C)	Mean annual total precipitation (mm)
Astoria (1997–2002)	2.7	7.1	14.8	1820.4
Bishop (1997–2002)	1252.4	3.0	23.6	108.3

Table 4. Monthly root mean square error of the daily mean temperature for Astoria, Oregon, USA, using three methods to determine the daily mean temperature. More details about these procedures are given in Weiss & Hays (2005)

Month	Root mean square error for daily mean temperature		
	Max/Min (°C)	Weighted (°C)	CERES (°C)
Jan	0.63	0.67	0.63
Feb	0.60	0.66	0.61
Mar	0.54	0.62	0.54
Apr	0.63	0.49	0.64
May	0.56	0.51	0.57
Jun	0.51	0.43	0.52
Jul	0.62	0.41	0.64
Aug	0.61	0.43	0.64
Sep	0.82	0.60	0.86
Oct	0.69	0.65	0.70
Nov	0.72	0.67	0.73
Dec	0.61	0.57	0.61

Table 5. Monthly root mean square error of the daily mean temperature for Bishop, California, USA, using three methods to determine the daily mean temperature. More details about these procedures are given in Weiss & Hays (2005)

Month	Root mean square error for daily mean temperature		
	Max/min (°C)	Weighted (°C)	CERES (°C)
Jan	1.07	1.02	1.16
Feb	0.84	0.87	0.87
Mar	1.06	0.92	0.96
Apr	1.23	1.11	1.07
May	1.59	1.22	1.41
Jun	1.72	1.25	1.53
Jul	1.88	1.28	1.68
Aug	1.61	1.21	1.40
Sep	1.21	1.06	1.05
Oct	0.87	1.00	0.86
Nov	0.97	1.15	1.03
Dec	1.09	0.94	1.22

it is very difficult to identify how exactly the specific method was meant to be applied.’

ALGORITHMS

Minimum and maximum air temperatures are important input parameters into many crop simulation models. Often these temperatures are used in non-linear algorithms. A question that should be addressed in the development of a non-linear algorithm is whether the temperatures be averaged first to form a single daily mean value and then the response calculated or should the response be calculated for each temperature and then averaged in a sequential manner? Weiss & Hays (2005) evaluated five different methods to calculate daily mean air temperature (Appendix 1) and used these different temperature methods in a non-linear algorithm of plant development based on Streck *et al.* (2003; Appendix 2). This non-linear algorithm was evaluated over a wide range of locations; elevation, temperature and precipitation

data for the two extreme locations, Astoria, Oregon, USA and Bishop, California, USA are given in Table 3. There was little difference in the daily mean air temperatures calculated by the different methods as evaluated by the root mean square error (RMSE) (Tables 4 and 5). The differences in magnitude of the RMSE indicate the variability of the two climates at these locations. For example, the July RMSE value for the max/min method was 0.62 °C for Astoria and 1.88 °C for Bishop. The empirical coefficient in this non-linear algorithm of plant development, the maximum development rate, was determined based on the daily mean air temperature of the 24-hourly temperature values. There were differences in the phenological responses from the non-linear algorithm when using any sequential approach when compared with the original algorithm (Table 6). For Astoria, the differences in the simulated days between the original algorithm and any sequential method to reach a specific stage were between 0.5 to 2.2 days. Even though the calculation methods from the original algorithm

Table 6. *The mean differences in days between simulated phenological development using different temperature methods. More details about these methods are given in Weiss & Hays (2005)*

Method	Astoria, Oregon, USA (days)	Bishop, California, USA (days)
Sequential hourly	1.0	9.3
Sequential max/min	2.2	39.8
Sequential weighted	0.5	4.8
Sequential mean 3 hour	0.8	9.0
Sequential CERES	0.7	12.5
Max/min	-0.3	1.8
Weighted	0.2	-0.7
Mean 3 hour	0.0	0.0
CERES	-0.5	1.2

were not followed, the simulated results were very good. This result implies that any calculation method works reasonably well in a relatively uniform climate, which implies that the 'correct' answer is obtained for the wrong reasons. On the other hand, for the more extreme climate found in Bishop, the differences between the simulated days to reach a specific stage were between 4.8 and 39.8 days. Not following the procedures in the original algorithm resulted in poor simulations for this type of climate. For either location, using a single mean temperature resulted in simulations that differed by 0.5 to 1.8 days. These results do not imply that the sequential approaches are inappropriate; just that the mean temperature method used to determine empirical coefficients in a non-linear algorithm must be consistently used in all applications especially in development of model algorithms and comparison with observed data for model evaluation. Although a specific parameter was used in Weiss & Hays (2005), the results are relevant to any non-linear algorithm containing empirically determined coefficients.

In simulating the developmental response of photosensitive plants, the ability to predict daylength is essential. Daylength can be defined in six ways depending upon the angle of the sun with the horizon (Forsythe *et al.* 1995). The US government definition of sunrise and sunset is when the rim of the sun is 0.8333° below the horizon. The value of 0.8333 degrees is a combination of the radius of the sun (in degrees as seen from the earth) plus 34 minutes for the value adopted for the refraction of light through the atmosphere. Daylength based on civil, nautical, and astronomical twilight occurs when the sun is higher than 6 , 12 and 18° below the horizon, respectively. Many modellers assume photosensitive plants respond to light beginning at civil twilight. To further complicate this issue, it is likely that species have

different minimum thresholds for photosensitive responses. The CROPGRO model (Boote *et al.* 1998) uses a definition of daylength based on 0 degrees, i.e. when the sun is on the horizon. The difference in daylength between this definition and civil twilight is about 1 h at 41° latitude. This difference in daylength depends upon the location of the sun and the horizon; 0 and 6° below the horizon may influence the simulation of development in CROPGRO. Forsythe *et al.* (1995) found that the solar declination algorithm in CERES-Wheat (Jones & Kiniry 1986) was in error, which could result in varying errors in the computation of daylength depending upon latitude and day of year ranging from no error at the equator to 170 min at 60° N latitude between day of year 148–201 (28 May–20 July). When Forsythe *et al.* (1995) corrected for this error in CERES-Wheat, they found that the simulated time to terminal spikelet varied by one week between the US government definition of daylength and civil twilight. These differences in calculated daylength may not be as serious as anticipated since these values are multiplied by empirical coefficients to simulate the duration of a developmental phase, the value of the empirical coefficient compensating for the problem associated with the calculation of daylength. This calculation, involving compensating errors, is probably valid if the empirical coefficients and the calculated daylength are based on the same observational data set. Differences in the choice and application of daylength algorithms may produce widely differing results, paralleling the confusion in application of the algorithm for thermal time highlighted by McMaster & Wilhelm (1997).

The above discussion is based upon the assumption that the topography is uniform with no nearby obstructions. For conditions of non-uniform topography, the definitions of sunrise and sunset would have to be adjusted for each unique situation. That is, traditional definitions of sunrise and sunset, and therefore daylength, should be adjusted for sites in mountainous areas.

In addition to the different definitions of daylength that can be used, there are different types of algorithms that can be used to simulate a photoperiod response, Fig. 1. One response is based on two straight lines, which is used in SOYGRO (Boote *et al.* 1998). A negative exponential relationship can also be used to describe the relationship between photoperiod and a 0–1 response (Angus *et al.* 1981). Both relationships require two inputs, a critical photoperiod, which in the case of short day plants is the length of daylight above which there is no response. In Fig. 1, the critical photoperiod is about 17 h. The second parameter is a shape factor, which in the case of the two straight lines relationship is the slope of the line that intersects the x-axis. A similar definition of the shape factor applies to the negative exponential relationship, how rapidly the response decreases with

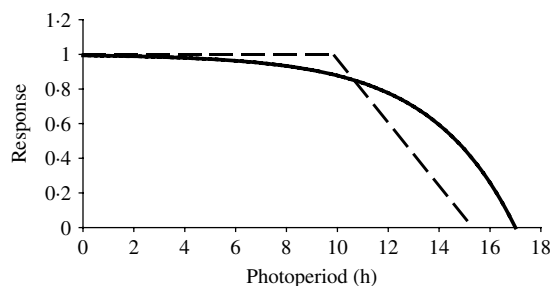


Fig. 1. Comparison of photoperiod response functions (0–1) based on two straight lines (dashed lines) and a continuous curve (solid line).

increasing photoperiod in a non-linear fashion. As photoperiod increases the differences in response between the two relationships increase until it is about 0.20 at 11 h, the straight line relationship with a value of 1.00, while the negative exponential approach has a value of 0.80. At about 13 h, the negative exponential relationship begins to over-predict compared with the straight-line relationship. Results from these two relationships are used with empirically determined coefficients to provide reasonable responses, although the negative exponential relationship was based on field measurements.

CONCLUSIONS

The intent of the present paper was not to serve as a guide on avoiding errors, but rather to stimulate thinking and discussion of the types of potential errors (variation may be a better term) that can complicate our attempts to develop, construct, evaluate, and use crop simulation models and determine how accurately they describe responses observed in the field. Each of these steps has the potential to cause

disagreement between observed and simulated values. The present authors' hope is that the current paper highlights enough examples so that those using models think broadly about causes for agreement or disagreement between field observation and simulation results. We realize that the thoughts expressed in this paper are not completely original. No doubt others have thought of at least some of these examples; they may even have additional examples; they may even have better examples. Listing examples of how observed and simulated data may disagree is easy. Finding ways to avoid or compensate for the limitation of both field observations and simulation results is the difficult and an ongoing challenge. We have purposely avoided providing suggested solutions for the examples given in this paper. Solutions are situation- and objective-specific. As one goes from generalities to specifics, that well-worn phrase, the devil is in the details, is applicable.

As the *Journal of Agricultural Science, Cambridge* enters its second century of publishing, crop simulation models will be increasingly used at all levels to organize and understand the relationships between physical, chemical and biological processes, genetics, and management practices in crop production. We anticipate that the *Journal of Agricultural Science, Cambridge* will remain a primary outlet for these types of papers. Thorough reporting by authors, assessment and comment by reviewers, and oversight by editors will greatly help in clearly communicated objectives, methods and results. Together, these efforts will minimize the types of misunderstandings, misinterpretation and errors cited here.

A joint contribution of the University of Nebraska Agricultural Research Division and USDA-ARS, Lincoln, NE. Journal Series No. 14517. This research was supported in part by funds provided through the Hatch Act.

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APPENDIX

APPENDIX 1

The five methods used to calculate daily mean air temperature (\bar{T}).
 Hourly

$$\bar{T} = \left(\sum_{i=1}^{i=24} T_i \right) / 24 \tag{1}$$

where i is the hour
 T_i is the hourly mean air temperature for hour i ($^{\circ}\text{C}$)

Weighted

$$\bar{T} = (T_{0700} + T_{1400} + 2 * T_{2100}) / 4 \tag{2}$$

where T_{0700} is the hourly mean air temperature for 0700 local time ($^{\circ}\text{C}$)
 T_{1400} is the hourly mean air temperature for 1400 local time ($^{\circ}\text{C}$)
 T_{2100} is the hourly mean air temperature for 2100 local time ($^{\circ}\text{C}$)

Mean 3 hour

$$\bar{T} = \left(\sum_{i=1}^{i=8} T_{3i} \right) / 8 \tag{3}$$

where i is every 3 hours (0300, 0600, ... 2100, 2400 local time)
 T_3 is the 3 hour mean temperature for hour i ($^{\circ}\text{C}$)

CERES (Jones & Kiniry 1986)

$$\bar{T} = \left\{ \sum_{i=1}^{i=8} T_{ci} \right\} / 8 \tag{4}$$

where i is 1 to 8

$T_{ci} = T_{min} + tmfac_i (T_{max} - T_{min})$ ($^{\circ}\text{C}$)
 T_{min} is the daily minimum temperature ($^{\circ}\text{C}$)
 T_{max} is the daily maximum temperature ($^{\circ}\text{C}$)
 $tmfac_i = 0.931 + 0.114i - 0.0703i^2 + 0.0053i^3$;
 for $i = 1$ to 8

Max/min

$$\bar{T} = (T_{min} + T_{max}) / 2 \tag{5}$$

where T_{min} is the daily minimum temperature ($^{\circ}\text{C}$)
 T_{max} is the daily maximum temperature ($^{\circ}\text{C}$)

APPENDIX 2

The temperature component of a non-linear algorithm for plant development.

$$f(T) = \frac{2(T - T_n)^{\alpha} (T_{opt} - T_n)^{\alpha} - (T - T_n)^{2\alpha}}{(T_{opt} - T_n)^{2\alpha}}; \tag{1}$$

if $T_n \leq T \leq T_x$

$$f(T) = 0; \text{ if } T < T_n \text{ or } T > T_x \tag{2}$$

$$\alpha = \ln 2 / \ln [(T_x - T_n) / (T_{opt} - T_n)] \tag{3}$$

$$R_{dev} = R_{max} f(T) \tag{4}$$

where T is the temperature ($^{\circ}\text{C}$)
 T_n is the minimum cardinal temperature
 T_x is the maximum cardinal temperature
 T_{opt} is the optimum cardinal temperature
 R_{max} is the maximum development rate

More details about this algorithm are given in Streck *et al.* (2003).